Hard-spin mean-field theory of a three-dimensional stacked-triangular-lattice system

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Closed form solutions to the hard-spin mean-field equations are constructed for the three-dimensional stacked triangular system. The phase diagram of this system is examined. The free energy of the system is calculated within the same approximation to identify the thermodynamically stable states in the phase diagram. A second-order phase transition line is found to exist for very small values of the external field. Our results display the details of the structure of the multicritical region within the hard-spin mean-field theory approximation.

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I. INTRODUCTION

Hard-spin mean-field theory has been developed recently [1] to improve upon the conventional mean-field theory. It was first applied to frustrated systems by Netz and Berker [2], and self-consistent equations were solved by a Monte Carlo implementation. Netz and Berker have also presented an iterative solution of hard-spin mean-field equations for three-dimensional stacked triangular system without a magnetic field [3]. The method is very successful in its application to frustrated systems.

The stacked-triangular-lattice antiferromagnetic Ising model has been studied by Monte Carlo [4] and renormalization group methods [5]. In the present work, closed form solutions to the hard-spin mean-field equations are constructed for the three-dimensional stacked triangular system with or without a finite magnetic field. This method enables a solution to the hard-spin mean-field equations with numerically minimum error. A second-order phase transition line is found to exist for very small values of the external field. The detailed structure of the multicritical region is also presented. Hard-spin mean-field theory has proven to be as effective as the other successful methods for this system.

II. MODEL

The Hamiltonian H of the system for ferromagnetic coupling between layers may be written as

$$-\beta H = -J\sum_{\langle i,j\rangle} S_iS_j + J'\sum_{\langle i,j\rangle} S_iS_j + h\sum_i S_i \ , \quad (2.1)$$

where $\beta \equiv 1/k_B t$ (with k_B the Boltzmann constant and t the temperature), $J > 0$ is the antiferromagnetic coupling constant between nearest-neighbor spins in a layer corresponding to a triangular lattice, $J' > 0$ is the ferromagnetic coupling constant between nearest-neighbor spins in neighboring layers, h is the scaled external magnetic field, and $S_i = \pm 1$ are the classical spin variables. Based on the scaling (by $k_B t$) apparent in Eq. (2.1), one may parametrize the equation of state of the system through a unitless temperature variable $T = 1/J$ and the temperature independent variables J'/J and h/J. The summation in Eq. (2.1) then runs over a set of spins consistent with the definitions of these interaction constants.

In the system under consideration, three sublattices are expected to have different and uniform magnetizations. In hard-spin mean-field theory, the average of the hyperbolic tangent of effective field is estimated by a weighted average of this quantity. The weights are given by the probabilities for the configurations of the hard spins. A detailed description of the method may be found in the Ref. [1]. The symmetry of the system is preserved in the approximation by considering three nearest-neighbor spins on a layer exactly and by including the effects of all other neighboring spins through the effective fields corresponding to the hard-spin approximation.

Because of the summation over the three spins which belong to three sublattices, the symmetry in the exponential function is retained. A sum over all configurations of the three central spins and their "hard-spin" neighbors must be carried out in order to obtain the average. Hard-spin mean-field equations for the stacked-triangular-lattice case will be (there are three coupled equation for m_1, m_2, and m_3)

$$m_{1,2,3} = \sum_{\sigma_1,\sigma_2,\cdots,\sigma_{15}} \frac{(1+\sigma_1 m_i)}{2}\frac{(1+\sigma_2 m_i)}{2} \times \cdots \times \frac{(1+\sigma_{15} m_i)}{2} \times \frac{\sum_{S_{\{1,2,3\}}} S_{1,2,3}\exp(-\beta H[S_{\{1,2,3\}},\sigma_i])}{\sum_{S_{\{1,2,3\}}}\exp(-\beta H[S_{\{1,2,3\}},\sigma_i])} \ . \quad (2.2)$$

The explicit form of the Hamiltonian is

$$\begin{aligned}-\beta H[S_{\{1,2,3\}},\sigma_i] = & -J(\sigma_1+\sigma_2+\sigma_3+\sigma_4)S_1 - J(\sigma_4+\sigma_5+\sigma_6+\sigma_7)S_2 \\ & -J(\sigma_7+\sigma_8+\sigma_9+\sigma_1)S_3 - J(S_1S_2 - S_2S_3 - S_3S_1) \\ & +J'(\sigma_{10}+\sigma_{11})S_1 + J'(\sigma_{12}+\sigma_{13})S_2 + J'(\sigma_{14}+\sigma_{15})S_3 + h(S_1+S_2+S_3) \ , \end{aligned} \quad (2.3)$$

where sites $i = 1,2,3$ form an elementary triangle of the lattice and $\sigma_1, \sigma_2, \ldots, \sigma_{15}$ represent the 15 hard-spin sites neighboring this elementary triangle. Spins $\sigma_1, \sigma_2, \ldots, \sigma_9$ are antiferromagnetically coupled to an elementary triangle in the lattice (on the same layer) and spins $\sigma_{10}, \sigma_{11}, \ldots, \sigma_{15}$ are neighbors to the elementary triangle which are ferromagnetically coupled to it (on neighboring layers).

Free energy was calculated within the same approximation as in Ref. [6] in order to identify the stable phases of the system. The derivative of free energy with respect to β is evaluated using the hard-spin approximation

$$\frac{\partial f}{\partial \beta} = -\frac{\partial}{\partial \beta} \ln \sum_S \exp -\beta H = \langle H \rangle \approx \langle H \rangle_{\mathrm{HSMF}} \ , \quad (2.4)$$

where the angular brackets indicate ensemble averaging and the subscript HSMF indicates the hard-spin mean-field approximation. This quantity is then integrated with respect to β, starting from a high temperature reference point, to the point of interest on the phase diagram, in order to determine the free energy at this point. The resultant free energy is used to differentiate the stable phase with zero magnetic field.

III. CALCULATIONS

The coupled equations given in Eq. (2.2) are solved numerically. In general, it is possible to find unstable and indeed unphysical solutions to these nonlinear equations.

A Landau-Ginzburg mean-field theory argument implies that two different ordered phases are possibly stable in this system. Two of the three sublattice magnetizations may be in the same direction with the same magnitude and the third one in the opposite direction with a different magnitude (hereafter referred to as the "up-up-down" phase). Alternatively, one of the sublattice magnetizations could be zero and the others in the two opposite directions (hereafter referred to as the "up-zero-down" phase). But a strong magnetic field can destroy these phases and all magnetizations will be in the same direction as the magnetic field (this is essentially the paramagnetic phase referred to as the "up-up-up" phase).

The thermodynamic degrees of freedom of the system are the external magnetic field and temperature, which define the magnetization phase diagram. The differentiation between stable and unstable phases may be done through a free energy comparison.

All stable phases are shown in Fig. 1. A similar dia-

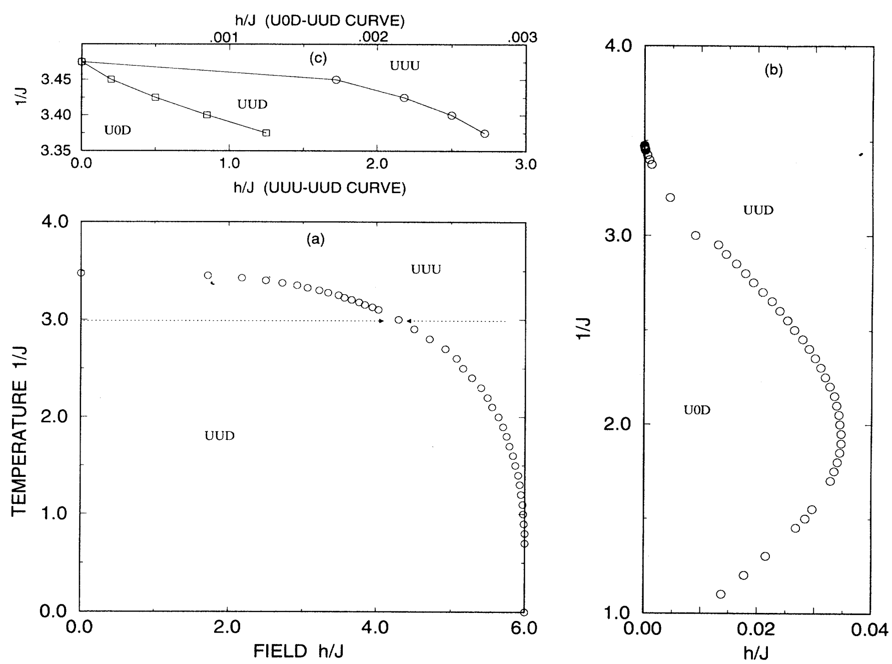

FIG. 1. Phase diagram of the three-dimensional stacked-triangular-lattice system. The sublattice magnetizations (i.e., phases) are abbreviated as follows: U, up; 0, zero; and D, down. (a) The first-order phase transition boundary. All points are calculated as shown in Fig. 2, which corresponds to the $T = 3$ case, shown with a dotted line. (b) The second-order phase transition boundary. The calculation is done as shown in Fig. 3. The up-zero-down phase continuously changes to the up-up-down phase. The boundary meets the zero-field line at zero temperature. (c) Region near the multicritical point. Note that the scale for the up-zero-down phase has been magnified 1000 times and lines have been added for visualization purposes.

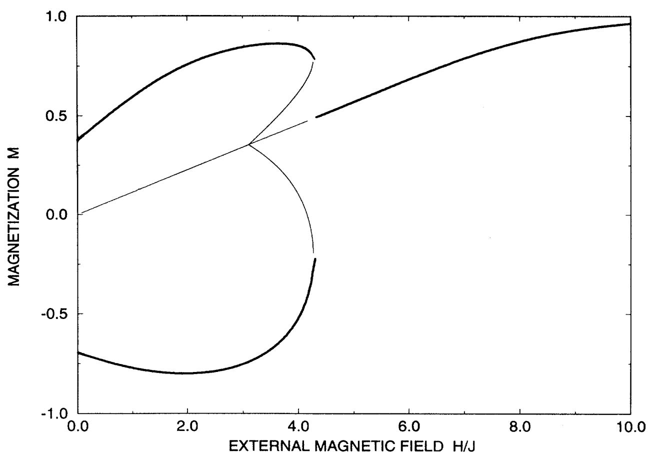

FIG. 2. Sublattice magnetizations for $T = 3$. The three magnetizations are equal for large fields. The stable solutions are indicated by the thick lines, corresponding to a first-order phase transition.

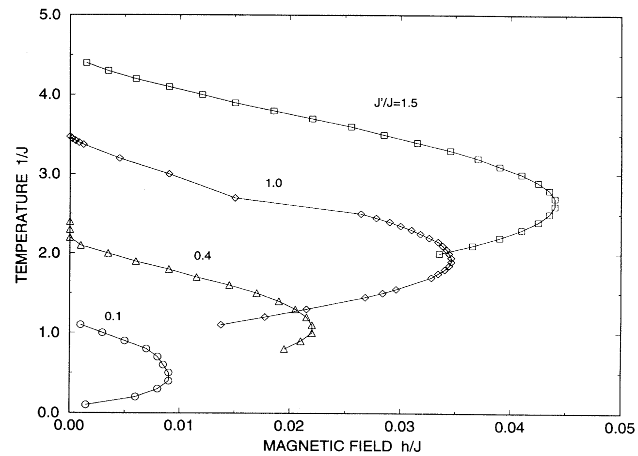

FIG. 4. Second-order transition lines for various values of J'/J. Indicated points on the curves correspond to values where computations were made. The boundaries meet the zero-field line at zero temperature.

gram has been given in the hard-spin Monte Carlo work of Netz and Berker [2]. The accuracy of our method of solution results in a more detailed structure in the phase diagram. For higher magnetic field values, the magnetizations of the sublattices are in the same direction as the external magnetic field. The magnitudes of three magnetizations are equal and depend on how strong the external magnetic field acting on the system is. The interaction of a spin with the external field dominates the phase diagram in this region. When the effect of the external magnetic field is sufficiently small, the contributions from other interaction terms start to appear.

For temperatures greater than $T > 3.475$ there is no phase transition for any value of magnetic field. There is a phase transition from the up-up-up phase to the up-up-down phase for $h/J < 6$. This is a first-order phase transition in the temperature interval $0 < T < 3.475$ (as in Fig. 2). If we further continue to decrease the external magnetic field in this temperature interval, there is a second-order phase transition from the up-up-down phase to the up-zero-down phase. The magnitude of the magnetization changes, as shown in Fig. 3, during this transition. The locus of critical points for different temperatures forms a second-order phase transition boundary. The implication of a second-order phase transition related to this curve is a result of the continuous bifurcation of the magnetizations near the critical points. (See Fig. 3.)

If the strength of the interlayer coupling is changed, considering various values of J'/J, it is observed that the second-order transition line extends up to smaller magnetic fields and to lower temperatures for smaller values

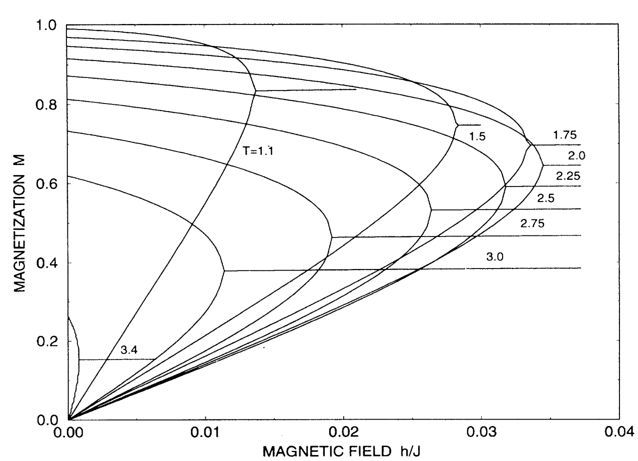

FIG. 3. Sublattice magnetizations for different temperatures during the transition from the up-up-down phase to the up-zero-down phase. The continuous change indicates a second-order phase transition.

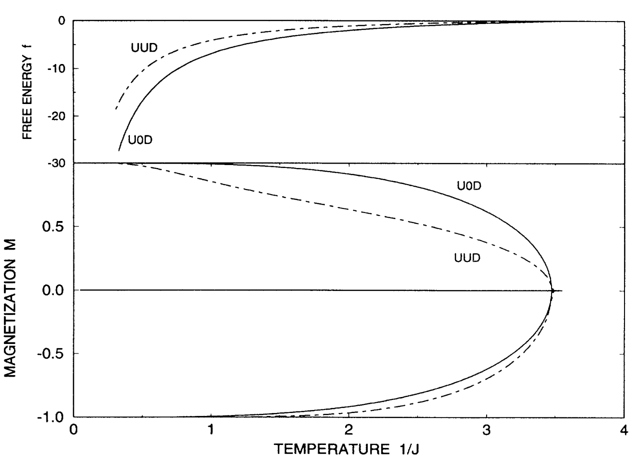

FIG. 5. Spontaneous sublattice magnetizations for zero magnetic field. The free energy corresponding to the two different phases is also shown at the top. (The smaller values correspond to the thermodynamically stable phase.) The up-zero-down phase is always stable for temperatures smaller than the critical temperature.

of J'/J (and vice versa for larger values of J'/J) compared to the $J'/J = 1$ case. This behavior is shown in Fig. 4. Without ferromagnetic coupling ($J' = 0$), the two-dimensional antiferromagnetic triangular lattice case is obtained, for which $h = 0$ corresponds to disorder [6].

The region near the point $T = 3.475$, $h = 0$ in the phase diagram is a multicritical region. This does not exist in two dimensions. The detailed structure of the multicritical region obtained in the present work is displayed in the phase diagram. In the Monte Carlo work of Heinonen and Petschek [4], indirect evidence for a tricritical point was found by an analysis of critical exponents. In the hard-spin Monte Carlo mean-field work of Netz and Berker [2], the resolution is not sufficient to identify the tricriticality behavior.

For zero external magnetic field the magnetization curve is shown in Fig. 5. The up-zero-down phase is found to be stable below the critical temperature based on free energy calculations. This is different from the previous work [3], which suggests a transition to the up-up-down phase above $T = 2.0$.

IV. CONCLUSIONS

A new second-order phase transition boundary has been observed with the help of the accurate closed form solutions of the hard-spin mean-field equations. The behavior of this transition is examined by looking at the various strength of the ferromagnetic coupling between the layers. In the limiting case, results corresponding to the two-dimensional triangular antiferromagnetic system are obtained. A detailed structure of the multicritical region, within the hard-spin mean-field approximation, was also presented. For zero magnetic field, free energy calculations show that the up-zero-down phase is thermodynamically stable below the critical temperature.

While our manuscript was in review, we were informed of a thesis [7] which contains some results consistent with those reported in this work.

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[1] R. R. Netz and N. Berker, J. Appl. Phys. **70**, 6074 (1991).
[2] R. R. Netz and A. N. Berker, Phys. Rev. Lett. **66**, 377 (1991).
[3] R. R. Netz and N. Berker, Phys. Rev. Lett. **67**, 1808 (1991).
[4] O. Heinonen and R. G. Petschek, Phys. Rev. B **40**, 9052 (1989).
[5] A. N. Berker, Gary S. Grest, C. M. Soukoulis, D. Blankschtein, and M. Ma, J. Appl. Phys. **55**, 2416 (1984).
[6] A. Kabakçıoglu, A. N. Berker, R. R. Netz, and C. Yalabik, Phys. Rev. E **49**, 2680 (1994).
[7] A. A. Naqvi, B.S. thesis, MIT, 1994.